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| Autore | Karthikeyan Muthukumarasamy |
| Titolo | Practical Chemoinformatics [[electronic resource] /] / by Muthukumarasamy Karthikeyan, Renu Vyas |
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| Edizione | [1st ed. 2014.] |
| Descrizione fisica | 1 online resource (XXI, 533 p. 621 illus.) |
| Disciplina | 542.85 |
| Soggetti | Cheminformatics<br>Chemistry, Physical and theoretical<br>Communication in chemistry<br>Computer Applications in Chemistry<br>Theoretical and Computational Chemistry<br>Documentation and Information in Chemistry |
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| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
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| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Open Source Tools, Techniques and Data in Chemoinformatics -- Chemoinformatics Approach for the Design and Screening of focused virtual libraries -- Machine Learning Methods in Chemoinformatics for Drug Discovery -- Docking and pharmacophore modeling for virtual screening -- Active site directed pose prediction programs for efficient filtering of molecules -- Representation, fingerprinting and modeling of chemical reactions -- Predictive methods for Organic Spectral data Simulation -- Chemical Text mining for Lead Discovery -- Integration of Automated Work flow in Chemoinformatics for drug discovery -- Cloud computing Infrastructure development for Chemoinformatics. |
| Sommario/riassunto | Chemoinformatics is equipped to impact our life in a big way mainly in the fields of chemical, medical and material sciences. This book is a product of several years of experience and passion for the subject written in a simple lucid style to attract the interest of the student community who wish to master chemoinformatics as a career. The topics chosen cover the entire spectrum of chemoinformatics activities (methods, data and tools). The algorithms, open source databases, tutorials supporting theory using standard datasets, guidelines, |

questions and do it yourself exercises will make it valuable to the academic research community. At the same time every chapter devotes a section on development of new software tools relevant for the growing pharmaceutical, fine chemicals and life sciences industry. The book is intended to assist beginners to hone their skills and also constitute an interesting reading for the experts.